

TAYLOR APPROXIMATIONS OF OPERATOR FUNCTIONS

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ABSTRACT. This survey on approximations of perturbed operator functions addresses recent advances and some of the successful methods.

1. INTRODUCTION

An active mathematical investigation of perturbed operator functions started in as early as 1950's, following a series of physics papers by I. M. Lifshits on the change of the free energy of a crystal due to appearance of a small defect. The latter research in physics gave birth to the Lifshits-Krein spectral shift function [31, 27, 28], which has become a fundamental object in perturbation problems of mathematical physics. Subsequent attempts to include more general perturbations than those in [27, 28] have resulted in consideration of higher order Taylor approximations of perturbed operator functions and introduction of Koplienko's higher order spectral shift functions [26, 36, 18, 42, 46, 44].

Approximation of operator functions also arises in problems of noncommutative geometry involving spectral flow (see, e.g., [8]) and spectral action functional (see, e.g., [16]). This investigation was initially carried out independently of the study of the spectral shift functions. However, a recent unified approach to the Lifshits-Krein spectral function and the spectral flow allowed to establish that these two objects essentially coincide [5]. Higher order Taylor formulas have been derived for spectral actions in [56], with restrictions on the operators relaxed in [54] by applying more universal perturbation theory techniques.

The proof of existence of the first order (Lifshits-Krein) spectral shift function, which is due to M. G. Krein, relied on the theory of analytic functions and was of a different nature than the proofs of the other mentioned results on the approximations of operator functions. An important object in higher order Taylor approximations is the Gâteaux derivative of an operator function. When the initial operator and the perturbation do not commute, the Gâteaux derivative is a complex object, whose complexity increases with the order of differentiation. Treatment of such derivatives and subsequent derivation of Taylor approximations was based on a delicate noncommutative analysis, which had been developing for some 60 years.

To proceed to a detailed discussion of the aforementioned and further results and methods, we need to fix some notation. We work with a pair of operators defined in a separable Hilbert space \mathcal{H} , denoting the initial operator H_0 and its perturbation V . The perturbation is always a bounded operator and, moreover, some summability

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restrictions are imposed either on V or H_0 . In some instances, H_0 is allowed to be unbounded, and we will consider only closed densely defined unbounded operators. For sufficiently nice scalar functions f , we consider the operator functions $f(H_0)$ and $f(H_0 + V)$ given by the functional calculus. We are interested in some scalar characteristics associated with perturbations that are calculated using traces (a canonical trace Tr , a Dixmier trace Tr_ω , a normal trace on a semi-finite von Neumann algebra τ , and, more generally, any trace $\tau_{\mathcal{I}}$ on a normed ideal \mathcal{I} continuous in the ideal norm).

We consider the remainders of the Taylor approximations

$$R_{n,H_0,V}(f) = f(H_0 + V) - \sum_{k=0}^{n-1} \frac{1}{k!} \left. \frac{d^k}{dt^k} \right|_{t=0} f(H_0 + tV),$$

where $n \in \mathbb{N}$ and the Gâteaux derivatives $\left. \frac{d}{dt} \right|_{t=0} f(H_0 + tV)$ are evaluated in the uniform operator topology. If the n -th order Gâteaux derivative is continuous on $[0, 1]$, then we have the integral representation for the remainder

$$R_{n,H_0,V}(f) = \frac{1}{(n-1)!} \int_0^1 (1-t)^{n-1} \frac{d^n}{dt^n} f(H_0 + tV) dt, \quad (1.1)$$

which can be proved by applying functionals in the dual space $(\mathcal{B}(\mathcal{H}))^*$ of the algebra of bounded linear operators on \mathcal{H} and reducing the problem to the scalar case. The questions we are interested in consist in establishing more specific properties of the remainders $R_{n,H_0,V}(f)$.

2. SCHATTEN CLASS PERTURBATIONS

In this section, we discuss Taylor approximations in the classical setting of perturbations belonging to the Schatten-von Neumann ideals of compact operators

$$S^\alpha = \{A \in \mathcal{B}(\mathcal{H}) : \|A\|_n := (\text{Tr}(|A|^\alpha))^{\frac{1}{\alpha}} < \infty\}, \quad \alpha \in [1, \infty)$$

(see, e.g., [50]). The operator functions under consideration come from either polynomials \mathcal{P} or the functions with nice Fourier transforms

$$\mathcal{W}_n = \{f : f^{(j)}, \widehat{f^{(j)}} \in L^1(\mathbb{R}), j = 0, \dots, n\}.$$

The class \mathcal{W}_n includes such widely used sets of functions as $C_c^{n+1}(\mathbb{R})$ and the rational functions in $C_0(\mathbb{R})$, which we denote by \mathcal{R} .

2.1. Spectral shift functions. As a joint finding of many investigations, we have the following representation for the Taylor remainders corresponding to self-adjoint perturbations of self-adjoint operators.

Theorem 2.1. *If $H_0 = H_0^*$ and $V = V^* \in S^n$, $n \in \mathbb{N}$, then there exists a unique real-valued function $\eta_n = \eta_{n,H_0,V} \in L^1(\mathbb{R})$ and a constant $c_n > 0$ such that*

$$\|\eta_n\|_1 \leq c_n \|V\|_n^n$$

and

$$\text{Tr} \left(f(H_0 + V) - \sum_{k=0}^{n-1} \frac{1}{k!} \left. \frac{d^k}{dt^k} \right|_{t=0} f(H_0 + tV) \right) = \int_{\mathbb{R}} f^{(n)}(t) \eta_n(t) dt, \quad (2.1)$$

for $f \in \mathcal{W}_n$.

The cases $n = 1$, $n = 2$, and $n \geq 3$ are due to [27] (see also [29]), [26], and [42], respectively. The formula (2.1) has been extended from \mathcal{W}_n to the Besov class $B_{\infty 1}^n(\mathbb{R})$ in [37], [38], and [3], respectively. Differentiability of operator functions in the setting most applicable to Theorem 2.1 is discussed in [39] and [6]. The results of [6, 39] can also be used to justify that the trace on the left hand side of (2.1) is well defined.

The function η_n provided by Theorem 2.1 is called the n -th order spectral shift function associated with the pair of operators $(H_0, H_0 + V)$. The name to η_1 was given by M. G. Krein and can be understood from I. M. Lifshits' formula

$$\eta_1(\lambda) = \text{Tr}(E_{H_0}((-\infty, \lambda))) - \text{Tr}(E_{H_0+V}((-\infty, \lambda)))$$

holding for H_0 and V finite matrices, where E_H denotes the spectral measure of H . A number of remarkable connections of the first-order spectral shift function to other objects of mathematical physics can be found in the brief survey [9]. More detailed discussion of the first order spectral shift function can be found in [12, 50, 57] and of the second order one in [23]. When a perturbation V is in the Hilbert-Schmidt class S^2 , the higher order spectral shift functions can be expressed via the lower order ones [18, 52]. The former are more sensitive to the displacement of the spectrum under perturbation, as demonstrated in [51, 53].

The question of validity of

$$\text{Tr}(f(H_0 + V) - f(H_0)) = \int_{\Omega} f'(t) \eta_1(t) dt, \quad (2.2)$$

was also investigated for non-self-adjoint operators H_0 and $H_0 + V$. Here the set $\Omega \subset \mathbb{C}$ is determined by H_0 and V . The trace formula (2.2) with $\Omega = \mathbb{T}$ (the unit circle) was proved in [28] for unitary operators H_0 and $H_0 + V$ such that $V \in S^1$. The case of arbitrary bounded operators H_0 and $H_0 + V$ differing by $V \in S^1$ is naturally harder than the case of self-adjoint operators. If H_0 and $H_0 + V$ are contractions, then (2.2) holds with $\Omega = \mathbb{T}$ and the function η_1 replaced by a finite complex-valued measure ν_1 , for every f analytic on a disc centered at zero of radius $r > 1$ [19]. Attempts to get more information about the structure of the measure ν_1 (for example, extract an absolutely continuous component) resulted in consideration of only selected pairs of contractions and brought to modification of (2.2) with passage to a more general type of integration. The relevant discussion (also for dissipative operators H_0 and $H_0 + V$) can be found in [1, 2, 30, 33, 34, 35, 47, 48, 49].

The higher order version of (2.2) for pairs of bounded operators has a more plausible formulation.

Theorem 2.2. *Let H_0 and $H_0 + V$ be contractions and assume that $V \in S^n$, $n \geq 2$. Then, there exists a function $\eta_n = \eta_{n, H_0, V}$ in $L^1(\mathbb{T})$ such that*

$$\text{Tr} \left(f(H_0 + V) - \sum_{k=0}^{n-1} \frac{1}{k!} \frac{d^k}{dt^k} \Big|_{t=0} f(H_0 + tV) \right) = \int_{\mathbb{T}} f^{(n)}(z) \eta_n(z) dz, \quad (2.3)$$

for $f \in \mathcal{P}$. Furthermore, there exists a constant $c_n > 0$ such that a function η_n satisfying (2.3) can be chosen so that

$$\|\eta_n\|_1 \leq c_n \|V\|_n^n. \quad (2.4)$$

The case $n = 2$ for H_0 and $H_0 + V$ unitaries, where the derivative is evaluated along a multiplicative path of unitaries instead of $t \mapsto H_0 + tV$, is due to [36] (with later extension of the class of functions f in [38]) and for arbitrary pairs of contractions H_0 and $H_0 + V$ joined by the path $t \mapsto H_0 + tV$ is due to [46]. The case $n \geq 3$ is established in [44]. The spectral shift function η_n satisfying Theorem 2.2 is determined uniquely only up to an analytic term (that is, the equivalence class of η_n in the quotient space $L^1(\mathbb{T})/H^1(\mathbb{T})$ is uniquely determined). Theorem 2.2 can be extended to more general functions f . In particular, (2.3) with $n = 2$ is established for analytic functions f in [19], as discussed in Subsection 3.3 for more general traces.

2.2. Proof strategy. The proofs of Theorems 2.1 and 2.2 are very subtle and technically involved, so we will give only a flavor of some basic ideas. For simplicity we assume that $\|H_0\| \leq 1$, $\|H_0 + V\| \leq 1$, $V \in S^n$, and $f \in \mathcal{P}$. Then our goal is the formula

$$\mathrm{Tr}(R_{n,H_0,V}(f)) = \int_{\mathbb{T}} f^{(n)}(z) \nu_n(z) dz, \quad (2.5)$$

where ν_n is a finite measure, with total variation bounded by

$$\|\nu_n\| \leq c_n \|V\|_n^n. \quad (2.6)$$

From the integral representation for the remainder (1.1), we derive

$$\mathrm{Tr}(R_{n,H_0,V}(f)) = \frac{1}{(n-1)!} \int_0^1 (1-t)^{n-1} \mathrm{Tr} \left(\left. \frac{d^n}{ds^n} \right|_{s=t} f(H_0 + sV) \right) dt.$$

Thus, if we prove

$$\sup_{t \in [0,1]} \left| \frac{1}{n!} \mathrm{Tr} \left(\left. \frac{d^n}{ds^n} \right|_{s=t} f(H_0 + sV) \right) \right| \leq c_n \|V\|_n^n \cdot \|f^{(n)}\|_\infty, \quad (2.7)$$

then application of the Hahn-Banach theorem and the Riesz representation theorem for the dual space of $C(\mathbb{T})$ implies existence of a measure ν_n satisfying (2.5) and (2.6).

For $n = 1$, we have

$$\mathrm{Tr} \left(\left. \frac{d}{ds} \right|_{s=t} f(H_0 + sV) \right) = \mathrm{Tr}(f'(H_0 + tV)V),$$

which in case of f a polynomial follows from the straightforward calculation of the derivative and some combinatorics. Applying the Hölder and von Neumann inequalities then implies (2.7) with $n = 1$ and $c_1 = 1$. This reasoning does not allow to establish the absolute continuity of ν_1 (which was established in [27]), but it can be generalized to apply to the higher order case. If, in addition, we take H_0 and V to be self-adjoint, then application on the spectral theory allows to derive an explicit formula for ν_1 , as it was done in [10].

Apart from the case of commuting H_0 and $V \in S^2$, we do not have the convenient equality $\text{Tr} \left(\frac{d^2}{ds^2} \Big|_{s=t} f(H_0 + sV) \right) = \text{Tr}(f''(H_0 + tV)V^2)$. However, since the set function $A_1 \times A_2 \mapsto \text{Tr}(E_{H_0+tV}(A_1)VE_{H_0+tV}(A_2)V)$, where A_1, A_2 are Borel subsets of \mathbb{R} , uniquely extends to a measure on \mathbb{R}^2 with total variation $\|V\|_2^2$, we have

$$\text{Tr} \left(\frac{d^2}{dt^2} \Big|_{s=t} f(H_0 + sV) \right) = \int_{\mathbb{R}^2} (f')^{[1]}(\lambda_1, \lambda_2) \text{Tr}(E_{H_0+tV}(d\lambda_1)VE_{H_0+tV}(d\lambda_2)V)$$

(see, e.g., [53, Theorem 3.12]), which along with the estimate for the divided difference $\|(f')^{[1]}\|_\infty \leq \|f''\|_\infty$ implies (2.7) with $n = 2$ and $c_2 = \frac{1}{2}$.

When $n \geq 3$, the set function $A_1 \times \dots \times A_n \mapsto \text{Tr}(E_{H_0+tV}(A_1)V \dots E_{H_0+tV}(A_n)V)$ can fail to extend to a measure of finite variation on \mathbb{R}^n (see [18, Section 4]). This is one of the reasons suggesting that the case $n \geq 3$ requires much more delicate (noncommutative) analysis of operator derivatives than the case $n < 3$.

Pioneering estimates for norms of n -th order operator derivatives are attributed to Yu. L. Daleckii and S. G. Krein [17]. In [17], $H_0 = H_0^*$ and $V = V^* \in \mathcal{B}(\mathcal{H})$, a scalar function f belongs to $C^{2n}(\mathbb{R})$, and the estimates depend on the size of the spectrum of the operator H_0 . Development of the Birman-Solomyak double operator integration (see, e.g., [11]) and subsequent multiple operator integration (see [39] and also [6]) resulted in significant improvement of the estimates for operator derivatives. It follows from [39] that for $H_0 = H_0^*$ and $V = V^* \in S^n$,

$$\sup_{t \in [0,1]} \left| \text{Tr} \left(\frac{d^n}{ds^n} \Big|_{s=t} f(H_0 + sV) \right) \right| \leq c_n \|f\|_{B_{\infty 1}^n(\mathbb{R})} \cdot \|V\|_n^n,$$

where $f \in B_{\infty 1}^n(\mathbb{R})$; however, the norm $\|f\|_{B_{\infty 1}^n(\mathbb{R})}$ is greater than the norm $\|f^{(n)}\|_{L^\infty(\mathbb{R})}$. The powerful estimates (2.7) are established in the following theorems.

Theorem 2.3. ([44]) *If $\|H_0\| \leq 1$, $\|H_0 + V\| \leq 1$, and $n \in \mathbb{N}$, then there exists a constant $c_n > 0$ such that for every $f \in \mathcal{P}$ the following estimates hold.*

(i) *If $\beta > n$ and $V \in S^\beta$, then*

$$\sup_{t \in [0,1]} \left\| \frac{d^n}{ds^n} \Big|_{s=t} f(H_0 + sV) \right\|_{\frac{\beta}{n}} \leq c_n \|V\|_\beta^n \cdot \|f^{(n)}\|_{L^\infty(\mathbb{T})}.$$

(ii) *If $V \in S^n$, then*

$$\sup_{t \in [0,1]} \left| \text{Tr} \left(\frac{d^n}{ds^n} \Big|_{s=t} f(H_0 + sV) \right) \right| \leq c_n \|V\|_n^n \cdot \|f^{(n)}\|_{L^\infty(\mathbb{T})}.$$

Theorem 2.4. ([42]) *If $H_0 = H_0^*$, $V = V^*$, and $n \in \mathbb{N}$, then there exists a constant $c_n > 0$ such that for every $f \in \mathcal{W}_n$ the following estimates hold.*

(i) *If $\beta > n$ and $V \in S^\beta$, then*

$$\sup_{t \in [0,1]} \left\| \frac{d^n}{ds^n} \Big|_{s=t} f(H_0 + sV) \right\|_{\frac{\beta}{n}} \leq c_n \|V\|_\beta^n \cdot \|f^{(n)}\|_{L^\infty(\mathbb{R})}.$$

(ii) If $V \in S^n$, then

$$\sup_{t \in [0,1]} \left| \text{Tr} \left(\frac{d^n}{ds^n} \Big|_{s=t} f(H_0 + sV) \right) \right| \leq c_n \|V\|_n^n \cdot \|f^{(n)}\|_{L^\infty(\mathbb{R})}.$$

The proofs of Theorems 2.3 and 2.4 (and also analogous estimates for polylinear transformations more general than operator derivatives) include a subtle synthesis of advanced techniques from harmonic, functional, complex analysis and noncommutative L^p spaces as well as development of a novel approach to multiple operator integration. The principal two cases here are the ones of self-adjoints and unitaries, while the case of contractions reduces to the case of unitaries by applying the Sz.-Nagy-Foias dilation theory [55].

2.3. Operator Lipschitz functions. Derivation of the estimates of Theorems 2.3 and 2.4 was preceded by resolution of Krein's conjecture on whether every Lipschitz function on \mathbb{R} is operator Lipschitz. Detailed discussion of the problem, including references to partial results, can be found in [40, 45]; here we only state the concluding result and mention some generalizations.

Theorem 2.5. ([45]) *Let f be a Lipschitz function on \mathbb{R} . Then, for every $\alpha \in (1, \infty)$, there is a constant $c_\alpha > 0$ such that*

$$\|f(B) - f(A)\|_\alpha \leq c_\alpha \|B - A\|_\alpha \cdot \|f\|_{Lip},$$

for all $A = A^*$, $B = B^*$, defined in \mathcal{H} with $B - A \in S^\alpha$.

The best constant $c_\alpha \sim \frac{\alpha^2}{\alpha-1}$ is obtained in [15]. It is known that not every Lipschitz function is operator Lipschitz in S^1 and in $\mathcal{B}(\mathcal{H})$ (i.e., when $\alpha \in \{1, \infty\}$) [20, 21, 22]. Operator Lipschitzness of functions of normal operators and of functions of several variables is discussed in [4, 24].

3. SOME NATURAL GENERALIZATIONS

If a perturbation V is not compact and no additional restriction on H_0 is imposed, then the canonical trace Tr of $R_{n,H_0,V}(f)$ is not defined. Depending on the problem, one can consider another trace that is defined on $R_{n,H_0,V}(f)$ for rather general H_0 , V , and f , or impose extra restrictions on H_0 , f , and/or V to ensure $R_{n,H_0,V}(f) \in S^1$.

3.1. Compact resolvents and similar conditions. Perturbations that arise in the study of differential operators are multiplications by functions defined on \mathbb{R}^d , which are not compact operators. In this case, the condition $V \in S^n$ gets replaced by a restriction on the resolvent of the initial operator H_0 .

If H_0 equals the negative Laplacian $-\Delta$ and the operator V act as multiplication by a real-valued function in $L^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, then

$$(H_0 - zI)^{-1} - (H_0 + V - zI)^{-1} \in S^1, \quad z \in \mathbb{C} \setminus \mathbb{R} \quad (3.1)$$

(see, e.g., [12]). Due to the invariance principle for the first order spectral shift function (see, e.g., [12]), the problem for a pair of self-adjoint operators (H_0, V) satisfying (3.1) reduces to the problem for a pair of unitaries with difference in S^1 , and (2.1) with $n = 1$ holds for $f \in C_c^\infty(\mathbb{R}) \cup \mathcal{R}$, as established in [28]. In this case,

η_1 is an element of $L^1(\mathbb{R}, \frac{1}{1+t^2}dt)$. Existence of the first order spectral shift function under more general resolvent conditions is discussed in [25, 58].

If $H_0 = -\Delta$ and V is a multiplication by a real-valued function in $L^2(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, then instead of the condition (3.1), we have

$$(I + H_0^2)^{-1/4}V \in S^2 \quad (3.2)$$

(see, e.g., [43]). It is established in [26] that for a pair of self-adjoint operators (H_0, V) satisfying (3.2), there exists $\eta_2 \in L^1(\mathbb{R}, \frac{1}{1+t^2}dt)$ such that the trace formula (2.1) with $n = 2$ holds for $f \in \mathcal{R}$. A modified trace formula is obtained in [43] for a pair (H_0, V) satisfying $(I + H_0^2)^{-1/2}V \in S^2$. The proofs are based on multiple operator integration techniques developed to partly compensate for the lack of the invariance principle under the assumption (3.2).

In perturbation problems of noncommutative geometry, typical assumptions on the operators are that the resolvent of H_0 is compact and $V \in \mathcal{B}(\mathcal{H})$. The following result is obtained in [54], relaxing assumptions on H_0 and V made in [56].

Theorem 3.1. *Let $H_0 = H_0^*$ be defined in \mathcal{H} and have compact resolvent and let $V = V^* \in \mathcal{B}(\mathcal{H})$. Let $\{\mu_k\}_{k=1}^\infty$ be a sequence of eigenvalues of H_0 counting multiplicity and let $\{\psi_k\}_{k=1}^\infty$ be an orthonormal basis of the respective eigenvectors. Then, for each function $f \in C_c^{n+1}(\mathbb{R})$, with $n \in \mathbb{N}$,*

$$\begin{aligned} & \text{Tr}(f(H_0 + V)) - \text{Tr}(f(H_0)) \\ &= \sum_{p=1}^{n-1} \frac{1}{p} \sum_{i_1, \dots, i_p} (f')^{[p-1]}(\mu_{i_1}, \dots, \mu_{i_p}) \langle V\psi_{i_1}, \psi_{i_2} \rangle \cdots \langle V\psi_{i_p}, \psi_{i_1} \rangle + \text{Tr}(R_{H_0, f, n}(V)), \end{aligned}$$

where

$$\text{Tr}(R_{H_0, f, n}(V)) = \mathcal{O}(\|V\|^n).$$

Moreover, the trace formula (2.1) with $f \in C_c^3(\mathbb{R})$ is established in [5] for $n = 1$ (this is also discussed in the next subsection) and, under the additional assumption $(I + H_0^2)^{-1/2} \in S^2$, in [54] for $n = 2$. The respective spectral shift functions η_1 and η_2 are locally integrable.

Taylor asymptotic expansions and spectral distributions have also been considered in the study of pseudodifferential operators (see, e.g., [13]).

3.2. Operators in a semifinite von Neumann algebra. Let \mathcal{M} be a semifinite von Neumann algebra of bounded linear operators defined on \mathcal{H} and let τ be a semifinite normal faithful trace τ on \mathcal{M} . (The definitions can be found in, e.g., [32].) Note that $(\mathcal{B}(\mathcal{H}), \text{Tr})$ is one of examples of (\mathcal{M}, τ) . Let H_0 be either an element of \mathcal{M} or an unbounded closed densely defined self-adjoint operator affiliated with \mathcal{M} (that is, all the spectral projections of H_0 are elements of \mathcal{M}). The perturbation V is taken to be a bounded element of the noncommutative L^p -space associated with (\mathcal{M}, τ) , that is,

$$V \in \mathcal{L}^n = \{A \in \mathcal{M} : \|A\|_n := \tau(|A|^n)^{\frac{1}{n}} < \infty\}, \quad n \in \mathbb{N}.$$

Theorem 3.2. *If $H_0 = H_0^*$ is affiliated with \mathcal{M} and $V = V^* \in \mathcal{L}^n$, $n \in \mathbb{N}$, then there exists a unique real-valued function $\eta_n = \eta_{n, H_0, V} \in L^1(\mathbb{R})$ and a constant $c_n > 0$ such that*

$$\|\eta_n\|_1 \leq c_n \|V\|_n^n$$

and

$$\tau \left(f(H_0 + V) - \sum_{k=0}^{n-1} \frac{1}{k!} \frac{d^k}{dt^k} \Big|_{t=0} f(H_0 + tV) \right) = \int_{\mathbb{R}} f^{(n)}(t) \eta_n(t) dt, \quad (3.3)$$

for $f \in \mathcal{W}_n$.

The case $n = 1$ was established first for a bounded operator H_0 in [14] and then for an unbounded operator in [7]. The case $n = 2$ is due to [18, 52] and $n \geq 3$ is due to [42]. The strategy of the proof is as described in Subsection 2.2; this strategy can be implemented because noncommutative L^p -spaces have much in common with Schatten ideals (see, e.g., [41]).

The first order spectral shift function for a pair of τ -Fredholm operators differing by a τ -compact perturbation is known to coincide with the spectral flow [5, Theorem 3.18]. It is also established in [5] that (3.3) with $n = 1$ holds for H_0 having τ -compact resolvent. (In the case $(\mathcal{M}, \tau) = (\mathcal{B}(\mathcal{H}), \text{Tr})$, a τ -compact operator is merely a compact operator.)

Theorem 3.3. ([5]) *If $H_0 = H_0^*$ is affiliated with \mathcal{M} and has a τ -compact resolvent and if $V = V^* \in \mathcal{M}$, then, for $f \in C_c^3((a, b))$,*

$$\tau(f(H_0 + V)) = \tau(f(H_0)) + \int_{\mathbb{R}} f'(\lambda) \tau(E_{H_0}((a, \lambda]) - E_{H_0+V}((a, \lambda])) d\lambda.$$

Analogues of (3.3) with $n = 1$ and $n = 2$ for pairs of arbitrary (non-self-adjoint) operators in \mathcal{M} differing by a perturbation $V \in \mathcal{L}^n$ are obtained in [19]. As to the case $n \geq 3$, the results of Theorem 2.4 can be extended to pairs of operators in \mathcal{M} by applying dilation of contractions in \mathcal{M} to unitary operators in semi-finite von Neumann algebras constructed in [19].

3.3. General traces. The canonical trace Tr is widely used, but it is not the most “typical” trace. The distinctive feature of Tr is that it is normal, i.e., has the property of monotonicity. A continuous trace on a normed ideal of compact operators in $\mathcal{B}(\mathcal{H})$ other than S^1 has a singular component, which vanishes on finite rank operators. Detailed discussion of traces and applications of singular traces to classical and noncommutative geometry can be found in [32].

Let \mathcal{M} be a semifinite (von Neumann) factor and \mathcal{I} a symmetrically normed ideal of \mathcal{M} with norm $\|\cdot\|_{\mathcal{I}}$. (The definitions can be found, e.g., in [19, 32].) Let $\tau_{\mathcal{I}}$ be a trace on \mathcal{I} bounded with respect to the ideal norm $\|\cdot\|_{\mathcal{I}}$. Examples of $(\mathcal{I}, \tau_{\mathcal{I}})$ include (S^1, Tr) , (\mathcal{L}^1, τ) , where τ is the normal faithful semifinite trace on \mathcal{M} , and $(\mathcal{L}^{(1, \infty)}, \text{Tr}_{\omega})$, where $\mathcal{L}^{(1, \infty)}$ denotes the dual Macaev ideal and Tr_{ω} the Dixmier trace on it corresponding to a generalized limit ω on $\ell^{\infty}(\mathbb{N})$.

The following results are obtained in [19].

Hypotheses 3.4. Consider a set Ω , a closed, densely defined operator H_0 affiliated to \mathcal{M} , an operator $V \in \mathcal{I}$ and a space \mathcal{F} of functions that satisfy one of the following assertions.

- (i) $\Omega = \text{conv}(\sigma(H_0) \cup \sigma(H_0 + V))$, $H_0 = H_0^* \in \mathcal{M}$, $V = V^*$, $\mathcal{F} = C^3(\mathbb{R})$;
- (ii) $\Omega = \mathbb{R}$, $\text{Im}(H_0) \geq 0$, $\text{Im}(H_0 + V) \geq 0$, and

$$\mathcal{F} = \text{span} \{ \lambda \mapsto (z - \lambda)^{-k} : k \in \mathbb{N}, \text{Im}(z) < 0 \};$$

- (iii) $\Omega = \mathbb{T}$, $\|H_0\| \leq 1$, $\|H_0 + V\| \leq 1$, and \mathcal{F} is the set of all functions that are analytic on discs centered at 0 and of radius strictly larger than 1.

Theorem 3.5. Let Ω , H_0 , V and \mathcal{F} satisfy Hypotheses 3.4. Then, there exists a (countably additive, complex) measure $\nu_1 = \nu_{1,H_0,V}$ on Ω such that

$$\|\nu_1\| \leq \min \{ \tau_{\mathcal{I}}(|\text{Re}(V)|) + \tau_{\mathcal{I}}(|\text{Im}(V)|), \|V\|_{\mathcal{I}} \}$$

and

$$\tau_{\mathcal{I}}(f(H_0 + V) - f(H_0)) = \int_{\Omega} f'(\lambda) \nu_1(d\lambda),$$

for all $f \in \mathcal{F}$. If Hypotheses 3.4(i) are satisfied, then the measure ν_1 is real and unique.

When $\mathcal{I} = S^1$, the measure ν_1 is absolutely continuous, but when \mathcal{I} is the dual Macaev ideal (with the Dixmier trace), the measure ν_1 can be of any type [19, Theorem 4.4]. Moreover, we do not have an explicit formula for ν_1 in case of a general trace $\tau_{\mathcal{I}}$. Derivation of an explicit formula for ν_1 in case $\mathcal{I} = S^1$, $H_0 = H_0^*$, and $V = V^*$ relies on the fact that $\text{Tr}(E_{H_0}(\cdot)V)$ is a (countably-additive) measure, while the set function $\text{Tr}_{\omega}(E_{H_0}(\cdot)V)$ can fail to be countably-additive (see [19, Section 3]).

As another consequence of singularity of Tr_{ω} (and, more generally, of every trace satisfying $\tau_{\mathcal{I}}(\mathcal{I}^2) = \{0\}$), we have the following linearization formula.

Theorem 3.6. Assume Hypotheses 3.4 and assume $\tau_{\mathcal{I}}(\mathcal{I}^2) = \{0\}$. Then,

$$\tau_{\mathcal{I}}(f(H_0 + V) - f(H_0)) = \tau_{\mathcal{I}}(f'(H_0)V).$$

Below we consider perturbations in the ideal $\mathcal{I}^{1/2} = \{A \in \mathcal{M} : |A|^2 \in \mathcal{I}\}$ and impose an additional natural assumption $\|AB\|_{\mathcal{I}} \leq \|A\|_{\mathcal{I}^{1/2}}\|B\|_{\mathcal{I}^{1/2}}$, which, in particular, holds for the ideals S^1 , \mathcal{L}^1 , and $\mathcal{L}^{(1,\infty)}$.

Hypotheses 3.7. Consider a set Ω , a closed, densely defined operator H_0 affiliated with \mathcal{M} , $V \in \mathcal{I}^{1/2}$ and a set \mathcal{F} of functions that satisfy one of the following assertions:

- (i) $\Omega = \mathbb{R}$, $\text{Im}(H_0) \geq 0$, $\text{Im}(H_0 + V) \geq 0$, and

$$\mathcal{F} = \text{span} \{ \lambda \mapsto (z - \lambda)^{-k} : k \in \mathbb{N}, \text{Im}(z) < 0 \};$$

- (ii) $\Omega = \mathbb{T}$, $\|H_0\| \leq 1$, $\|H_0 + V\| \leq 1$, and \mathcal{F} is the set of all functions that are analytic on discs centered at 0 and of radius strictly larger than 1.

Theorem 3.8. Let Ω , H_0 , V and \mathcal{F} satisfy Hypotheses 3.7. Then, there exists a (countably additive, complex) measure $\nu_2 = \nu_{2,H_0,V}$ on Ω such that

$$\|\nu_2\| \leq \frac{1}{2} \tau_{\mathcal{I}}(|V|^2)$$

and

$$\tau_{\mathcal{I}} \left(f(H_0 + V) - f(H_0) - \frac{d}{dt} \Big|_{t=0} f(H_0 + tV) \right) = \int_{\Omega} f''(\lambda) \nu_2(d\lambda),$$

for every $f \in \mathcal{F}$.

Theorem 3.9. *Suppose $\tau_{\mathcal{I}}(\mathcal{I}^{3/2}) = \{0\}$. Either assume Hypotheses 3.7 or else take $H_0 = H_0^* \in \mathcal{M}$, $V = V^* \in \mathcal{I}^{1/2}$, and $\mathcal{F} = C^4(\mathbb{R})$. Then, for every $f \in \mathcal{F}$,*

$$\tau_{\mathcal{I}} \left(f(H_0 + V) - f(H_0) - \frac{d}{dt} \Big|_{t=0} f(H_0 + tV) \right) = \frac{1}{2} \tau_{\mathcal{I}} \left(\frac{d^2}{dt^2} \Big|_{t=0} f(H_0 + tV) \right).$$

The major components in the proofs of Theorems 3.5 and 3.8 are analogs of the estimates (2.7), which hold due to the continuity of $\tau_{\mathcal{I}}$ with respect to $\|\cdot\|_{\mathcal{I}}$. However, presence of a singular component in the trace $\tau_{\mathcal{I}}$ requires more careful treatment of the operator derivatives than in the case of the normal trace Tr .

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